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THE STUDY OF ATOM-ATOM ELECTRON-MOLECULE & PHOTON-MOLECULE PROC--ETC(U)

OCT 81 J C BROWNE, E J SHIPSEY

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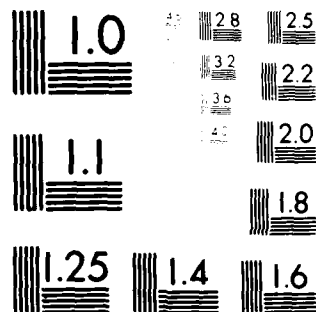
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<p>This research program has had two principal streams of activity. The first, and the major consumer of effort, has been the computation of cross-sections and rate coefficients for significant collision processes between light atoms and ions. The other stream of activity has been development of computational methods in collision mechanics. (continued)</p>		

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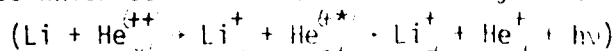
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The cross-section computations have on several occasions predicted experiments and/or corrected experimental errors. The prediction of the efficiency of the reaction $Cs + H \rightarrow Cs^+ + H^-$ was listed by the American Physical Society as a significant result for plasma physics in 1976. The first prediction of a process which could lead to a soft x-ray laser



was made in 1978. The population inversion predicted has since been experimentally validated.

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FINAL REPORT
TO
THE OFFICE OF NAVAL RESEARCH
ON
THE STUDY OF ATOM-ATOM ELECTRON-MOLECULE & PHOTON-MOLECULE PROCESSES
N00014-75-C-0498
for
April 1, 1975 - March 31, 1980

J. C. Browne and E. J. Shipsey
Departments of Computer Science and Physics
The University of Texas at Austin
Austin, Texas 78712

October 25, 1981

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1. ACCOMPLISHMENTS SUMMARY

This research program has had two principal streams of activity. The first, and the major consumer of effort, has been the computation of cross-sections and rate coefficients for significant collision processes between light atoms and ions. The other stream of activity has been development of computational methods in collision mechanics.

The cross-section computations have on several occasions predicted experiments and/or corrected experimental errors. The prediction of the efficiency of the reaction $\text{Cs} + \text{H} \rightarrow \text{Cs}^+ + \text{H}^-$ was listed by the American Physical Society as a significant result for plasma physics in 1976. The first prediction of a process which could lead to a soft x-ray laser ($\text{Li} + \text{He}^{++} \rightarrow \text{Li}^+ + \text{He}^{+*} \rightarrow \text{Li}^+ + \text{He}^+ + h\nu$) was made in 1978. The population inversion predicted has since been experimentally validated.

This period of work produced a substantial volume of publications in major journals. A total of 16 papers were published, 4 in the Physical Review, 7 in the Journal of Chemical Physics, 2 in the Journal of Physics B and 3 elsewhere.

2. RESEARCH AREA SUMMARIES

2.1 Computational Studies of Collision Processes

The overall theme of this research has been dynamics of colliding small atomic systems. The computational effort has been devoted mostly to the collisions of atoms with ions. The collision energy is low enough so that the colliding system is best described as a diatomic molecule. The electronic wavefunctions for the necessary set of states of the molecule are computed as a function

of internuclear separation and various matrix elements between different states evaluated to furnish the coupling elements driving the collision processes. The collision is thus treated in two steps; (i) a molecular electronic structure calculation and matrix element evaluation and (ii) solution of a coupled system of differential equations describing the nuclear motion in the framework of the adiabatic molecular state potential curves. The computational effort involved in (i) has been the principal activity of this group in Texas. The second part has been undertaken by our collaborator, R. E. Olson, while at S.R.I. International in California.

The calculation of electronic structure of diatomic molecules requires a set of complex computer programs. This program set has been in a process of evolution for many years in the molecular physics group and its implementation has been the subject of much study. Matrix element evaluation has also received much study in the past. A particular matrix element required for collisional processes was studied by Dr. Larry Lenamon who left shortly before this contract period began. The capabilities of the program set have been steadily improved over the period of this contract and their use made more convenient and user efficient.

The processes which have been studied have been selected to have both scientific and practical importance. The systems which have been investigated are



$$B^{+3}, C^{+4} + He \quad (3)$$

$$B^{+3}, C^{+4} + H \quad (13)$$

$$He^{++} + Li \quad (15).$$

The first of these $He^{+} + Ne$, was investigated at the request of a group of French experimentalists to aid in the interpretation of their results. The systems $B^{+3} + He$ and $C^{+4} + He$ are others in which experimental results were available prior to our computations. The $B^{+3} + He$ was actually the system in which we established the validity of our procedures, both by computer investigation and by comparison with experiment.

The original experiment on $C^{+4} + He$ ignored the possibility of two electron exchange. For this reason our calculation on this process which included both single and double charge exchange disagreed with the original experiment. When the experiment was repeated by other workers (4) essential agreement between our predictions and experiment was obtained.

Another system in which experiment was available prior to our calculations is the $H + Cs$ system. In this problem a simplified description of Cs was adopted and found to be satisfactory. This system has great practical importance for the creation of beams of H^{-} ions.

The remaining calculations all preceded experiment. The collisions involving H atoms are relevant to controlled fusion research. These collisions yield products in highly excited electronic states. Subsequent radiation represents an energy loss from the plasma. The $C^{+4} + H$ calculation disagreed with the experimental data which did exist. Various experimental problems

rendered the experimental results uncertain. When the experiment was repeated more carefully, under the guidance of predictions made by our calculations, the results were in essential agreement with our calculations. Further studies involving collisions between charged ions and H atoms have been carried out in the present research period with similar success and some studies still continue.

The remaining system, $\text{He}^{++} + \text{Li}$, was selected by R. E. Olson as presenting the best opportunity to yield products with a population inversion. The calculations confirmed this, and indeed experiments have been performed observing radiation in the far ultra-violet.

2.2 Computational Methods in Collision Mechanics

A second line of research investigated in this period has been computational methods in collision dynamics. High frequency approximations are well known in atomic collisions. There is a rich mathematical structure to such approximations and this has been investigated in (1), the third paper devoted to this purpose. The analysis yields simple methods for assessing the validity of such methods (away from turning points). The mathematical structure uncovered in the analysis has been applied in (2) to give a simple approximation for rate constants of certain chemical reactions. The analysis has also led to methods of partitioning systems of coupled differential equations. These methods have been applied to charge transfer collisions in (7&12). Finally, the one difficult region for approximation, the turning point region, has been investigated in (16) and suitable approximations have been devised and established through numerical example.

2.3 Other Work

There were also undertaken several other research projects of lesser duration and effort commitment. One of these was a collaboration with T. A. Green on a very thorough analysis of the molecular structure of HeH^+ (6&14). Another was a thorough computation of the dipole moment of HD (10). A third was a study of nuclear motion corrections to fixed nuclear molecular potential curves (9). Completion of work started in an earlier contract was represented by computation of the polarizability of the first excited state of the Li Atom (11).

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